**Supplementary materials**

**Table 1.** Hydrodynamic sizes, polydispersity indexes and zeta potentials of AgNTs, PNTs, ANTs, ENTs and AENTs in water, DMEM and DMEM with 10% FBS.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Environment | Sample | Hydrodynamic size (nm) | Polydispersity index | Zeta potential (mV) |
| Water | AgNTs | 85.34 | 0.363 | 36.03 |
| PNTs | 48.47 | 0.312 | 29.67 |
| ANTs | 54.23 | 0.343 | 30.12 |
| ENTs | 56.34 | 0.351 | 30.76 |
| AENTs | 59.73 | 0.334 | 31.33 |
| DMEM | AgNTs | 711.43 | 0.594 | -5.89 |
| PNTs | 327.84 | 0.382 | -6.09 |
| ANTs | 344.80 | 0.502 | -6.49 |
| ENTs | 269.34 | 0.487 | -6.25 |
| AENTs | 276.53 | 0.396 | -6.14 |
| DMEM with 10% FBS | AgNTs | 423.7 | 0.390 | -7.37 |
| PNTs | 77.82 | 0.381 | -10.13 |
| ANTs | 79.75 | 0.347 | -9.19 |
| ENTs | 83.23 | 0.336 | -9.36 |
| AENTs | 96.12 | 0.373 | -9.04 |

AgNTs: silver nanotriangles; PNTs: PEGylated silver nanotriangles; ANTs: AS1411-conjugated PEGylated silver nanotriangles; ENTs: EpDT3-conjugated PEGylated silver nanotriangles; AENTs: AS1411 and EpDT3-conjugated PEGylated silver nanotriangles; DMEM: Dulbecco’s modified Eagle’s medium; FBS: fetal bovine serum.

**Calculation of the photothermal conversion efficiency**

The photothermal conversion efficiency of AgNTs was determined according to a previous method [1]. The formula is given as following:

(1)

where *TMax* and *TSurr* are the maximum equilibrium temperature and the surrounding temperature, respectively. The temperature change (*TMax*-*TSur*r) of the AgNTs solution was 47.3 °C. *QDis* presents the heat dissipated from the light absorbed by the sample cell and it was measured to be approximately 30 mW with a quartz cuvette cell containing pure water. *I* is the laser power (1 W), and *A808*isthe absorbance (0.33) of the AgNTs solution at 808 nm. In order to determine photothermal conversion efficiency (*η*), all the parameters in equation (1) are known except heat transfer efficiency (*h*) and surface area of the container (*s*). A dimensionless driving force temperature *θ* and a sample system time constant *τs* are introduced to deduce *hs.* The equations are shown as following:

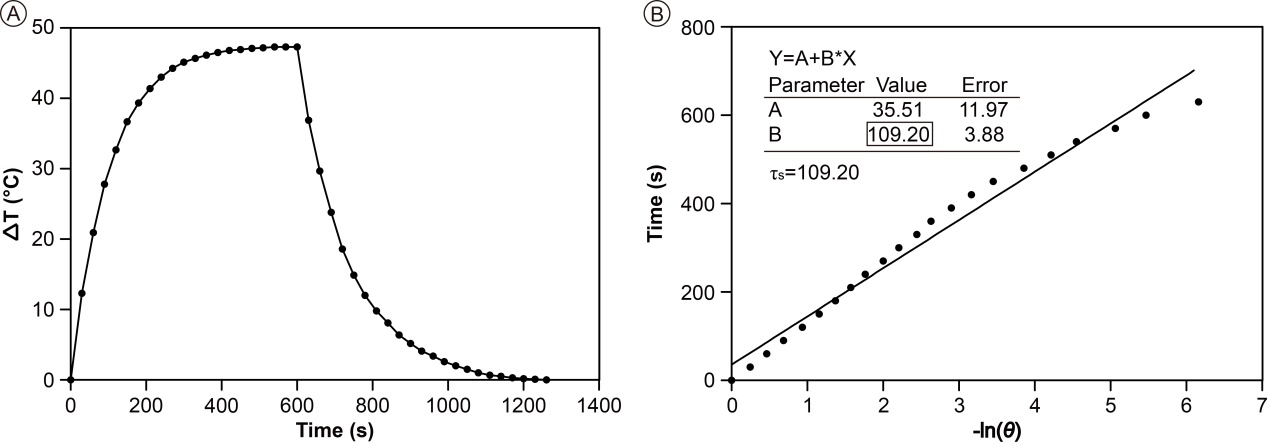
(2)

(3)

*△T (T-TSurr)* expresses the temperature change of the AgNTs solution response to 808 nm near-infrared laser (2 W/cm2) with the increase of time (Figure 1A). *τs* was calculated to be 109.2 s according to Figure 1(B). *hs* can be calculated using the following equation:

(4)

where *m* is the mass (0.15 g) and *Cp* is the heat capacity of water (4.2 J/g·°C). Thus, *hs* was determined to be 5.77 mW/°C and then the heat conversion efficiency (*η*) of AgNTs was calculated to be 45.7%.

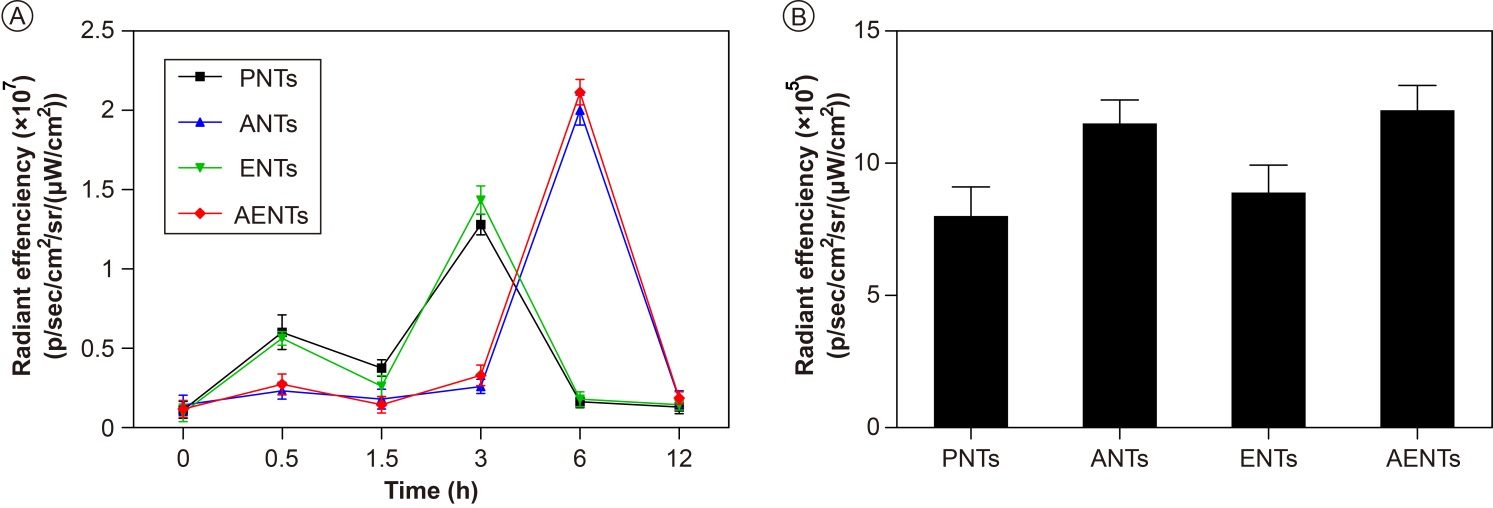


**Figure 1.** Calculation of the photothermal conversion efficiency. (A) Temperature change of AgNTs solution (10 μg/mL) under 808 nm near-infrared laser irradiation (2 W/cm2), in which the irradiation lasted for 600 s, and then the laser was shut off. (B) Linear time data versus -ln(*θ*) obtained from the cooling period of Figure 1A.

**Table 2.** IC50 values of PNTs, ANTs, ENTs and AENTs against MDA-MB-231 cells and breast CSCs

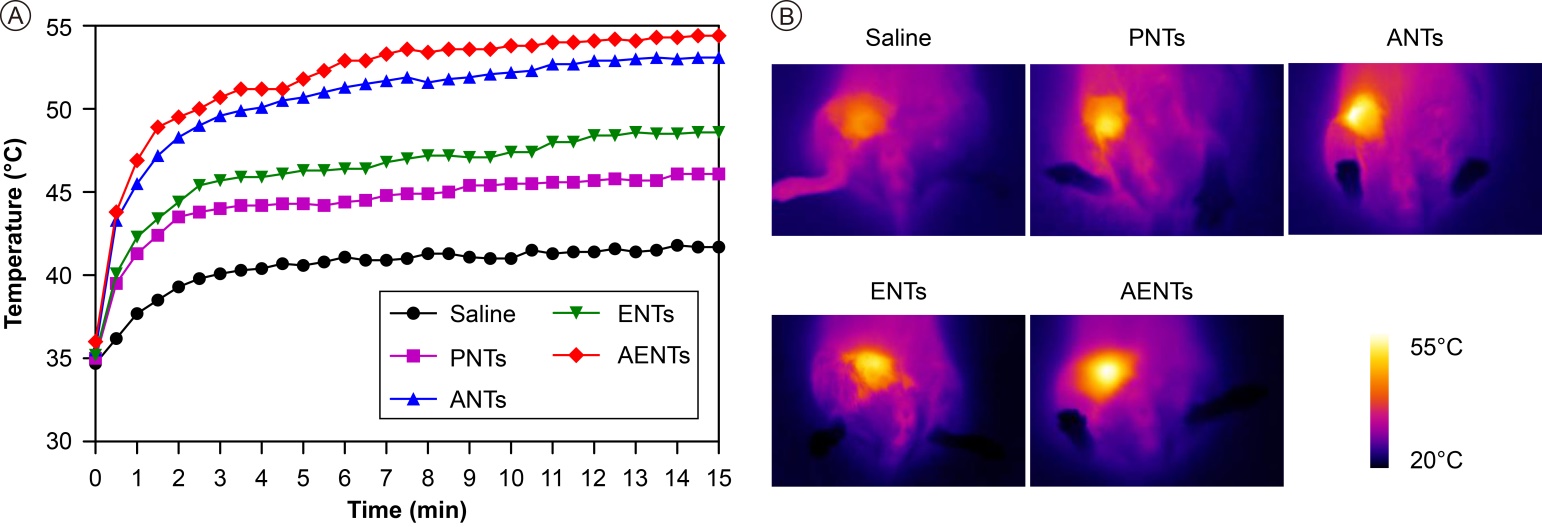
|  |  |  |
| --- | --- | --- |
| IC50 (μg/mL) | MDA-MB-231 | breast CSCs |
| PNTs | 116 | 86 |
| ANTs | 71 | 51 |
| ENTs | 108 | 59 |
| AENTs | 64 | 31 |

IC50: half maximal inhibitory concentration;PNTs: PEGylated silver nanotriangles; ANTs: AS1411-conjugated PEGylated silver nanotriangles; ENTs: EpDT3-conjugated PEGylated silver nanotriangles; AENTs: AS1411 and EpDT3-conjugated PEGylated silver nanotriangles; CSCs: cancer stem cells.



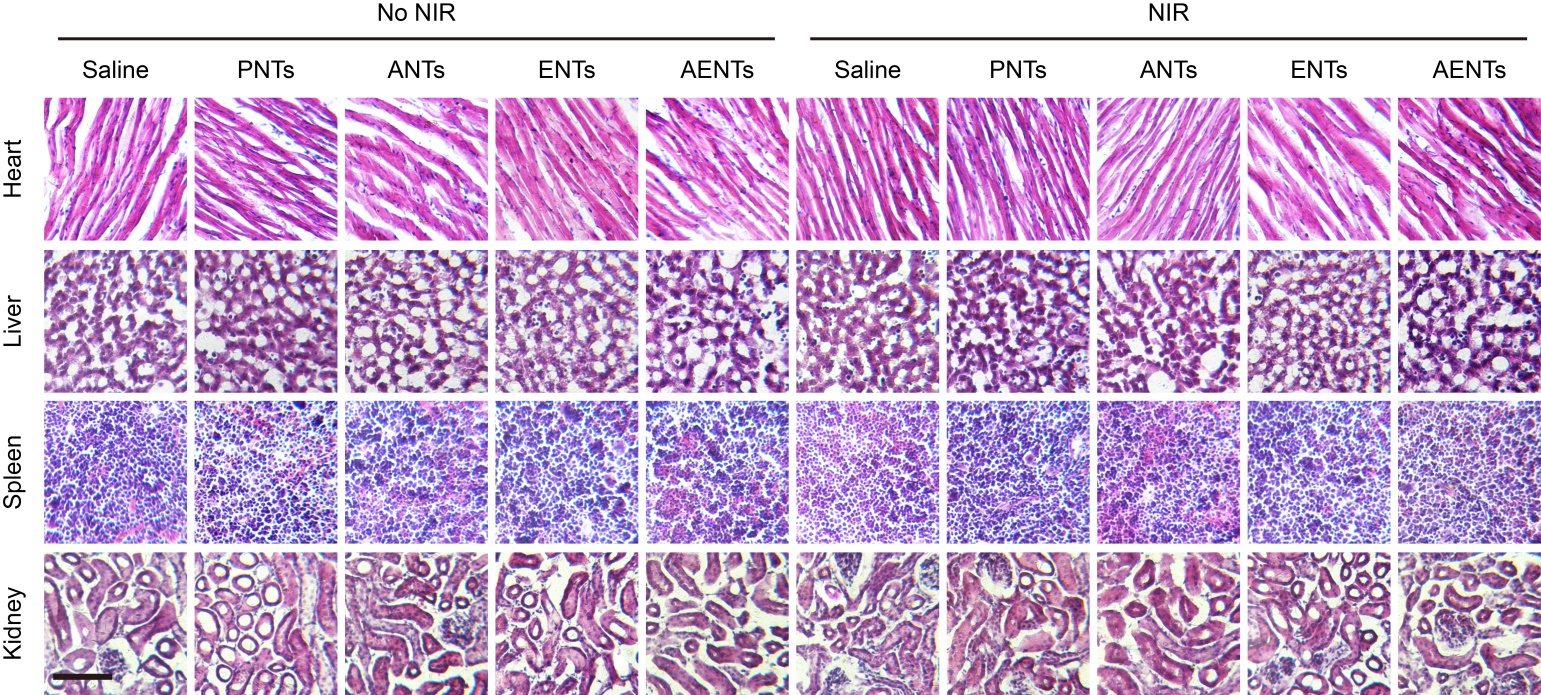
**Figure 2.** Quantitative analysis of Cy5-labeled PNTs, ANTs, ENTs or AENTs in tumor site and isolated tumors. (A) The fluorescence intensity of Cy5-labeled PNTs, ANTs, ENTs or AENTs in the tumor site at different times after the injection of nanomaterials via the tail vein. (B) The fluorescence intensity of Cy5-labeled PNTs, ANTs, ENTs or AENTs in the isolated tumors.

PNTs: PEGylated silver nanotriangles; ANTs: AS1411-conjugated PEGylated silver nanotriangles; ENTs: EpDT3-conjugated PEGylated silver nanotriangles; AENTs: AS1411 and EpDT3-conjugated PEGylated silver nanotriangles.



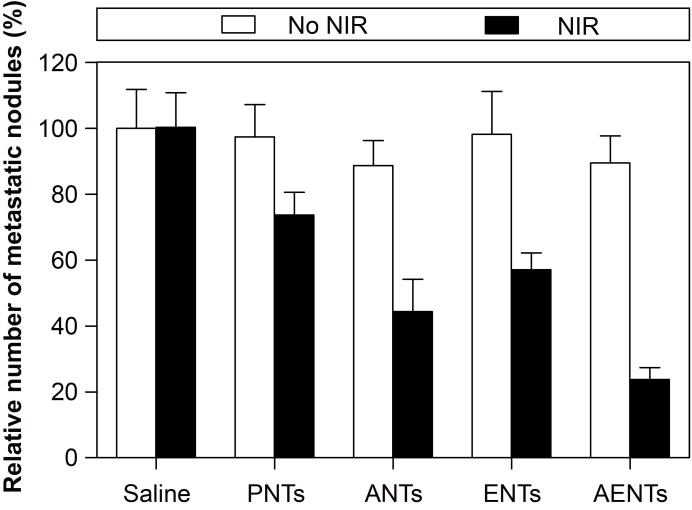
**Figure 3.** In vivo photothermal conversion effects of PNTs, ANTs, ENTs and AENTs. (A) Temperature changes and (B) infrared thermal images of tumor sites of breast cancer-bearing mice intravenously injected with 150 μL of saline or nanomaterials (PNTs, ANTs, ENTs or AENTs) at a dose of 4 mg/kg under 808 nm NIR laser irradiation (2 W/cm2,15 min).

PNTs: PEGylated silver nanotriangles; ANTs: AS1411-conjugated PEGylated silver nanotriangles; ENTs: EpDT3-conjugated PEGylated silver nanotriangles; AENTs: AS1411 and EpDT3-conjugated PEGylated silver nanotriangles; NIR: near infrared.



**Figure 4.** H&E staining images of heart, liver, spleen and kidney of breast cancer-bearing mice treated by intravenous injection of 150 μL of saline or nanomaterials (PNTs, ANTs, ENTs or AENTs) at a dose of 4 mg/kg with or without 808 nm NIR laser irradiation (2 W/cm2,15 min). Scale bar: 100 μm.

PNTs: PEGylated silver nanotriangles; ANTs: AS1411-conjugated PEGylated silver nanotriangles; ENTs: EpDT3-conjugated PEGylated silver nanotriangles; AENTs: AS1411 and EpDT3-conjugated PEGylated silver nanotriangles; NIR: near infrared.



**Figure 5.** Quantitative analysis of metastatic nodules in lungs of breast cancer-bearing mice treated by intravenous injection of 150 μL of saline or nanomaterials (PNTs, ANTs, ENTs or AENTs) at a dose of 4 mg/kg with or without 808 nm NIR laser irradiation (2 W/cm2, 15 min).

PNTs: PEGylated silver nanotriangles; ANTs: AS1411-conjugated PEGylated silver nanotriangles; ENTs: EpDT3-conjugated PEGylated silver nanotriangles; AENTs: AS1411 and EpDT3-conjugated PEGylated silver nanotriangles; NIR: near infrared.

References

1. Liu X, Li B, Fu F, *et al*. Facile synthesis of biocompatible cysteine-coated CuS nanoparticles with high photothermal conversion efficiency for cancer therapy. *Dalton. Trans*. 43(30), 11709–11715 (2014).